1,5-Dimethyl-6-phenyl-1,6-dihydro-3-pyridinecarbonitrile

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 6.18e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.01e-01

Confidence level: 4.02e-01

Nearest Neighbors from the Training Set

Image not found
5-methyl-1-phenylpyrrolidin-2-one
Measured: 1.43e-01
Predicted: 3.13e-01

Image not found
Heptachlor epoxide
Measured: 5.14e-07
Predicted: 3.52e-07

Image not found
Sparteine
Measured: 1.30e-02
Predicted: 8.29e-03

Image not found
Furilazole
Measured: 7.08e-04
Predicted: 7.48e-02